

Special Issue on
Computational Tools and Artificial Intelligence in Chemical Engineering

CALL FOR PAPERS

Chemical engineering systems and equipment represent highly complicated processes involving simultaneous momentum, heat, and mass transfer phenomena that occur at different length scales. Advanced mathematical models, optimization methods, and computational tools are essential for simulating complex chemical systems. Novel computational and simulation tools have been developed and used in the design, operation, and optimization of chemical engineering systems and equipment. The majority of computation tools require high computation costs and are based on mechanistic models.

Emerging methodologies enable the construction of hybrid data-driven models for process-product design and synthesis, and the integration of cutting-edge artificial intelligence (AI) technologies. Data-driven optimization algorithms are used for the optimization of more complex chemical systems, and AI-powered decision-making tools are now applied in chemical production planning and scheduling. While the integration of machine learning (ML) and computation tools has been previously limited, recent years have witnessed a significant improvement in AI-based research driven by increased data availability and computational resources. Computational tools have contributed to our fundamental understanding of chemical engineering systems, while ML facilitates the development of intelligent predictive models for the optimization and maintenance of chemical engineering systems.

The Special Issue welcomes studies on the application of innovative computational methods, optimization algorithms, and AI-driven approaches to solving complex problems in chemical process design, simulation, optimization, and control. In addition, we invite submissions highlighting the transformative impact of data-driven methodologies and machine-learning techniques on various aspects of chemical engineering. We welcome both original research and review articles.

Potential topics include but are not limited to the following:

- ▶ Application of computational tools in chemical engineering
- ▶ Mathematical modelling of chemical engineering processes using computational methods
- ▶ Process design and control using optimization algorithms
- ▶ Application of AI in chemical engineering
- ▶ Predictive analysis using different ML methods including neural networks
- ▶ Decision making using expert systems
- ▶ Process control and automation using fuzzy logic
- ▶ Optimization of processes using reinforcement learning (RL)
- ▶ Process safety analysis using probabilistic reasoning
- ▶ Nonlinear process dynamics and optimization using hybrid AI approaches, including neuro-fuzzy systems and physics-informed neural networks
- ▶ Effective prediction using emerging AI techniques, such as explainable AI (XAI), data augmentation, and transfer learning

Authors can submit their manuscripts through the Manuscript Tracking System at <https://review.wiley.com/submit?specialIssue=156855>.

Papers are published upon acceptance, regardless of the Special Issue publication date.

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